Zero modes of two-dimensional chiral p-wave superconductors

V. Gurarie and L. Radzihovsky
Department of Physics, University of Colorado, Boulder CO 80309
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We discuss fermionic zero modes in the two-dimensional chiral p-wave superconductors. We show quite generally, that without fine-tuning, in a macroscopic sample there is only one or zero of such Majorana-fermion modes depending only on whether the total vorticity of the order parameter is odd or even, respectively. As a special case of this, we find explicitly the one zero mode localized on a single odd-vorticity vortex, and show that, in contrast, zero modes are absent for an even-vorticity vortex. One zero mode per odd vortex persists, within an exponential accuracy, for a collection of well-separated vortices, shifting to finite $\pm E$ energies as two odd vortices approach. These results should be useful for the demonstration of the non-Abelian statistics that such zero-mode vortices are expected to exhibit, and for their possible application in quantum computation.

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Recently [1–3] there has been considerable interest in the structure of fermionic zero modes localized on vortices of a chiral spinless two-dimensional superconductor characterized by $p_x + ip_y$ order parameter. In part, it is stimulated by a proposal [1] that a ground state of such a superconductor (for a positive chemical potential) is similar to the Moore-Read (Pfaffian) quantum Hall state [4], thought to describe the $\nu = 5/2$ quantum Hall plateau [5]. Vortices (corresponding to the Laughlin quasihole-like excitations [6] in the Moore-Read state) in such a superconductor are thus expected to exhibit a degenerate set of zero modes separated from all other states by a gap, and to obey non-Abelian statistics [7], that may make them useful for a realization of a "topological quantum computer" [8] free of decoherence.

Many of the properties of these zero modes for a *single* vortex have already been discussed in the literature [1–3]. However, in our view an explicit discussion of the fate and robustness of the zero modes to, for example, a local deformation of the order parameter or in the presence of many vortices has not appeared in the literature. Such questions are of particular interest in view of recent proposals for experimental realization and manipulation of such non-Abelian states in two-dimensional superconductors, such as Sr_2RuO_4 [9], the $\nu = \frac{5}{2}$ plateau of the quantum Hall effect [10–12], and p-wave resonantly interacting atomic superfluids [2, 13].

In this Letter we show quite generally, that for a macroscopic sample (i.e., ignoring the boundary physics), without fine-tuning, strictly speaking there is only *one* or *zero* Majorana-fermion mode depending only on whether the total vorticity of the order parameter (in elementary vortex units of 2π) is *odd* or *even*, respectively. For a collection of well-separated vortices, within an exponential accuracy one zero mode per an isolated odd-vorticity vortex persists. As two of such vortices are brought closer together the corresponding pair of "zero" modes splits away to finite $\pm E$ (vortex-separation dependent) energies. Generically, even-vorticity vortices do not carry any zero modes.

Even in the odd-vorticity case, zero modes only exist for a *positive* chemical potential $\mu > 0$, consistent with the existence (absence) of a topological order in a weakly- (strongly-) paired ground state of a p-wave superconductor stable only for $\mu > 0$ ($\mu < 0$) [1, 14]. While a p-wave superconductor in a solid state context naturally obeys $\mu > 0$, in a Feshbach resonant atomic p-wave superfluid a chemical potential can be adjusted to be positive via an external magnetic field [13], a "knob" that can also be used to drive a topological quantum phase transition between a strongly- and weakly-paired superfluid ground states [1].

As a demonstration of a specific realization of this general connection between parity of vorticity and a number of zero modes, we compute the eigenfunction of the one zero mode localized on a single isolated odd-vorticity vortex, and show that zero modes are absent for an even-vorticity vortex. This symmetric vortex result is in agreement with a recent study in Ref. [3], but does not rely on a linearization of the fermion dispersion around a Fermi surface, and thereby allows us to access the nondegenerate (low chemical potential) regime realizable in tunable (via a Feshbach resonance [13]) atomic gas experiments. Our results then imply that such zero-modes, residing on isolated elementary vortices are always shifted to finite $\pm E$ energies when an even number of them come into proximity [1], with possible deleterious implications for a realization of non-Abelian statistics and quantum computation.

To demonstrate these results we begin by first discussing the properties of the solutions of generic Bogoliubov-de-Gennes (BdG) equations arising in a context of any superconductor. These coupled Schrödinger equations follow from the following Bardeen-Cooper-Schrieffer (BCS) Hamiltonian

$$H = \sum_{ij} \left(a_i^\dagger h_{ij} a_j - a_j h_{ij} a_i^\dagger + a_i \Delta_{ij} a_j + a_j^\dagger \Delta_{ij}^* a_i^\dagger \right), \quad (1)$$

where indices i, j label space (and in a spinful case, spin) coordinates of the fermion creation and annihilation operators $a_i^\dagger$, a_i. Their canonical anticommutation relations ensure that Δ_{ij} is an antisymmetric operator. Since H must be hermitian, so is h_{ij}, and the problem is equivalent to a study of the spectrum and eigenstates of a matrix

$$\mathcal{H} = \begin{pmatrix} h & \Delta \\ \Delta^\dagger & -h^T \end{pmatrix}. \tag{2}$$

This matrix possesses the following important symmetry property

$$\sigma_1 \mathcal{H} \sigma_1 = -\mathcal{H}^*, \tag{3}$$

where σ_1 is the first Pauli matrix acting in the 2 by 2 space of the matrix $\mathcal{H}$, Eq. (2). In the terminology of Ref. [15], the matrix $\mathcal{H}$ is said to belong to the symmetry class D. As a result of this property, it can be seen from

$$\mathcal{H}\sigma_1\psi^* = -\sigma_1\mathcal{H}^*\psi^* = -E\sigma_1\psi^* \tag{4}$$

that if ψ is an eigenvector of such $\mathcal{H}$ with the eigenvalue E, then $\sigma_1\psi^*$ is guaranteed to be an eigenvector with the eigenvalue $-E$. As a result, all nonzero eigenvalues of $\mathcal{H}$ come in $\pm E$ pairs. A special role is played by the zero eigenvectors of this matrix, referred to as zero modes. If ψ is a zero mode, $\sigma_1\psi^*$ is also a zero mode. Taking linear combinations $\psi + \sigma_1\psi^*$, $i(\psi - \sigma_1\psi^*)$ of these degenerate modes, we can always ensure the relation

$$\sigma_1\psi^* = \psi \tag{5}$$

for every zero mode. In the absence of other symmetries of $\mathcal{H}$ it is quite clear that generically there is nothing that protects the total number N_z of its zero modes under smooth changes of the Hamiltonian matrix that preserve its BdG form. However, since non-zero modes have to always appear in $\pm E$ pairs, as long as the symmetry property (3) is preserved by the perturbation the number of zero modes can only change by multiples of 2. Thus, while the number N_z of zero modes of the Hamiltonian (2) may change, this number will always remain either odd or even, with $(-1)^{N_z}$ a "topological invariant" [16, 17].

The value of this invariant is easy to establish if one observes that $\mathcal{H}$ is an even sized matrix, with an even number of eigenvalues. Since the number of non-zero modes must be even, this implies, quite generally that the number of zero modes is also even, $(-1)^{N_z} = 0$, and strictly-speaking the BdG Hamiltonian does not have any topologically protected zero modes. Furthermore, since zero modes must appear in pairs, there can only be an even number of accidental zero modes, which will nevertheless be generally destroyed by any perturbation of $\mathcal{H}$ (preserving its BdG structure Eq. (2)). We believe this observation was first made by N. Read [17].

The situation should be contrasted with that of the Dirac operators $\mathcal{D}$. Those operators, being generally of one of the chiral classes in the terminology of Ref. [15], obey the symmetry

$$\sigma_3\mathcal{D}\sigma_3 = -\mathcal{D}.$$

Thus if ψ is an eigenvector of $\mathcal{D}$ with the eigenvalue E, $\sigma_3\psi$ is an eigenvector with the eigenvalue $-E$. Thus, (after a suitable diagonalization) the zero modes of $\mathcal{D}$ must obey the relation

$$\sigma_3\psi_{L,R} = \pm\psi_{L,R}.$$

Namely, they are eigenstates of the σ_3 operator, with the "left" zero modes ψ_L coming with the eigenvalue $+1$, and the "right" zero modes ψ_R labelled by the eigenvalue -1. As the operator $\mathcal{D}$ is deformed, the number of zero modes changes, but the non-zero modes always appear in pairs, where one of the members of a pair has to be "left" and the other "right". Therefore, while the number of zero modes is not an invariant, the difference between the number of left and right zero modes is a topological invariant, determined (through the index theorem) by the monopole charge of the background gauge-field.

Contrast this with zero modes of $\mathcal{H}$, which obey the relation Eq. (5). Because of the complex conjugation on ψ, these zero modes cannot be split into "left" and "right". Indeed, even if we tried to impose $\sigma_1\psi^* = -\psi$, a simple redefinition of $\psi \to i\psi$ brings this relation back to Eq. (5). Thus, the most an "index theorem" could demonstrate in the case of the BdG problem, is whether there is 0 or exactly 1 zero mode. Moreover, since the BdG problem is defined by an even-dimensional Hamiltonian, generically there will not be any topologically protected zero modes [16, 17].

Yet it is quite remarkable that in the case of an isolated vortex of odd vorticity in a macroscopic sample (i.e., ignoring the boundaries) of a $p_x + ip_y$ superconductor of spinless fermions, there is exactly one zero mode localized on this vortex [1–3, 18]. To be consistent with above general property of the BdG Hamiltonian (namely, that the total number of zero modes must be even) another vortex is situated at the boundary of the system [1, 17], preserving the overall parity of the number of zero modes. Hence, although even in this odd-vorticity case the one zero mode is not protected topologically, able to hybridize with a vortex at a boundary of the sample, it survives (up to exponentially small corrections) only by virtue of being far away from the boundary (and from other odd-vorticity vortices).

To see this explicitly we consider the BdG equations for a two-dimensional $p_x + ip_y$ superconductor

$$\left(-\frac{\nabla^2}{2m} - \mu\right) u(\mathbf{r}) - \sqrt{\Delta(\mathbf{r})}\frac{\partial}{\partial \bar{z}}\left[v(\mathbf{r})\sqrt{\Delta(\mathbf{r})}\right] = Eu(\mathbf{r}),$$
$$\left(\frac{\nabla^2}{2m} + \mu\right) v(\mathbf{r}) - \sqrt{\Delta^*(\mathbf{r})}\frac{\partial}{\partial z}\left[u(\mathbf{r})\sqrt{\Delta^*(\mathbf{r})}\right] = Ev(\mathbf{r}). \tag{6}$$

Here $\Delta(\mathbf{r})$ is the order parameter of the superconductor, $z = x + iy$, $\bar{z} = x - iy$ are the two-dimensional complex coordinates, m is the fermion mass, and μ is the chemical potential. Eq. (6) is of course a particular case of the eigenvalue equation for a matrix of the form given in Eq. (2), with the vector ψ represented by

$$\psi = \begin{pmatrix} u \\ v \end{pmatrix}. \tag{7}$$

For a uniform (vortex-free) order parameter, $\Delta(\mathbf{r}) = \Delta_0$, it is easy to solve Eq. (6) in terms of plane waves, finding the spectrum

$$E_{\mathbf{k}} = \sqrt{\left(\frac{k^2}{2m} - \mu\right)^2 + |\Delta_0|^2 k^2}. \tag{8}$$

Since $E_{\mathbf{k}}$ has a gap for all $\mathbf{k}$ (with the exception of the critical point at $\mu = 0$ [1, 14]), consistent with above discussion, there are no zero modes of Eq. (6) in the absence of vortices.

Now consider a superconductor with a symmetric vortex of vorticity ℓ. The order parameter is then given by

$$\Delta(\mathbf{r}) = e^{i\ell\varphi} f^2(r), \tag{9}$$

where r, φ are the polar coordinates centered on the vortex and $f(r)$ is a real function of r that vanishes at small r. Then the BdG equations take the form

$$\begin{aligned} \left(-\frac{\nabla^2}{2m} - \mu\right) u - f(r) e^{\frac{i\ell\varphi}{2}} \frac{\partial}{\partial \bar{z}} \left[e^{\frac{i\ell\varphi}{2}} f(r) v \right] &= Eu, \\ \left(\frac{\nabla^2}{2m} + \mu\right) v - f(r) e^{-\frac{i\ell\varphi}{2}} \frac{\partial}{\partial z} \left[e^{-\frac{i\ell\varphi}{2}} f(r) u \right] &= Ev. \end{aligned} \tag{10}$$

Next we observe that for the case of a vortex of *even* vorticity, $\ell = 2n$, we can eliminate the phase dependence of Eq. (10) entirely . Indeed, making a transformation

$$u \to u e^{in\varphi}, \;\; v \to v e^{-in\varphi}. \tag{11}$$

leads to equations

$$\begin{aligned} \left(-\frac{\nabla^2}{2m} + \frac{n^2}{2mr^2} - \mu\right) u - \frac{in}{mr^2}\frac{\partial u}{\partial \varphi} - f(r)\frac{\partial}{\partial \bar{z}}\left[f(r) v\right] &= Eu, \\ \left(\frac{\nabla^2}{2m} - \frac{n^2}{2mr^2} + \mu\right) v - \frac{in}{mr^2}\frac{\partial v}{\partial \varphi} - f(r)\frac{\partial}{\partial z}\left[f(r) u\right] &= Ev. \end{aligned} \tag{12}$$

Now we note that these equations are topologically equivalent to the BdG equations without any vortices. Indeed, the only difference between these equations and those for a uniform condensate is the presence of the terms $2in/r^2[\partial/\partial\varphi]$, n^2/r^2, and $f(r)$ that is a constant at large r and vanishes in the core of the vortex for $r < r_{\rm core}$. We can imagine smoothly deforming these equations to get rid of the first two terms (for example, by replacing them with $\alpha\left(n^2/r^2 - 2in/r^2[\partial/\partial\varphi]\right) u$ and taking α from 1 to 0), and smoothly deforming $f(r)$ into a constant equal to its asymptotic value at large r; in order to be smooth, the deformation must preserve the BdG structure Eq. (2) and the vorticity of the order parameter. These equations then become equivalent to Eq. (6) for a constant, vortex-free order parameter $\Delta(\mathbf{r}) = \Delta_0$ with an exact spectrum Eq. (8), that for $\mu \neq 0$ clearly does not exhibit any zero modes.

As Eqs. (12) are smoothly deformed, in principle it is possible that for a particular deformation some of its eigenstates will become zero modes (although, as demonstrated above, this can only happen in $\pm E$ pairs, leading to an even number of these). However, these modes will not be topologically protected, and even a small deformation of, say, the order parameter shape $f(r)$ will destroy these modes. We note that this argument easily accommodates vortices that are not symmetric, as those can be smoothly deformed into symmetric ones without changing the topologically protected parity of N_z. The conclusion is that generically there are no zero modes in the presence of an isolated vortex of even vorticity.

In fact, if any doubts remain, it is also possible to directly demonstrate the absence of zero modes in Eq. (12), simply by following the arguments parallel to those given after Eq. (20). However, the arguments presented above are more general and robust, and can be used to establish the claim even for non-symmetric even-vorticity vortices.

The situation is drastically different if the vorticity of a vortex is *odd*, i.e., $\ell = 2n - 1$. Indeed, in that case the transformation Eq. (11) cannot entirely eliminate such vortex from the equations (even with the help of a smooth deformation), leaving at least one fundamental unit of vorticity. This thereby guarantees at least one zero mode localized on the odd-vorticity vortex. To see this, recall that due to the condition Eq. (5) together with the definition Eq. (7), the zero mode satisfies

$$u = v^*. \tag{13}$$

Combining this with the transformation Eq. (11), we find the equation for the zero mode

$$\begin{aligned} -f(r) e^{-\frac{i\varphi}{2}} \frac{\partial}{\partial \bar{z}} \left[e^{-\frac{i\varphi}{2}} f(r) u^* \right] &= \\ \left(\frac{\nabla^2}{2m} - \frac{n^2}{2mr^2} + \mu\right) u + \frac{in}{mr^2}\frac{\partial u}{\partial \varphi}&. \end{aligned} \tag{14}$$

We look for a solution to this equation in terms of a spherically symmetric real function $u(r)$. This gives

$$-\frac{1}{2m}u'' - \left(\frac{f^2}{2} + \frac{1}{2mr}\right) u' - \left(\frac{f^2}{4r} + \frac{ff'}{2} - \frac{n^2}{2mr^2}\right) u = \mu u. \tag{15}$$

A transformation

$$u(r) = \chi(r) \exp\left(-\frac{m}{2}\int_0^r dr' \; f^2(r')\right) \tag{16}$$

brings this equation to the more familiar form

$$-\frac{\chi''}{2m} - \frac{\chi'}{2mr} + \left(m\frac{f^4(r)}{8} + \frac{n^2}{2mr^2} \right) \chi = \mu\chi. \qquad (17)$$

This is a Schrödinger equation for a particle of mass m which moves with angular momentum n in a potential $mf^4/8$ that is everywhere positive. We observe that this potential vanishes at the origin, and quickly reaches its asymptotic bulk value f_0 away from the origin. Then for $\mu > mf_0^4/8$, there always exist a solution to this equation finite at the origin and at infinity. Moreover, if $\mu < mf_0^4/8$, then the solution finite at the origin will diverge at infinity as

$$\chi \sim e^{r\sqrt{m^2 \frac{f_0^4}{4} - 2m\mu}}. \qquad (18)$$

Combining this with Eq. (16), we observe that $u(r)$ remains a bounded function at infinity as long as $\mu > 0$. Thus the conclusion is, there exist a zero mode as long as $\mu > 0$. For the special case of the $n = 0$ vortex of vorticity -1, the small and large r asymptotics of the solution we found here was discussed recently in Ref. [2].

In the simplest London approximation of a spatially uniform condensate with $f(r) = f_0$ for all r except inside an infinitesimally small core, the zero mode localized on an isolated odd-vorticity vortex is simply given by

$$u(r) = \begin{cases} J_n\left(r\sqrt{2\mu m - m^2\frac{f_0^4}{4}}\right) e^{-\frac{m}{2}f_0^2 r}, & \text{for } \mu > m\frac{f_0^4}{8}, \\ I_n\left(r\sqrt{m^2\frac{f_0^4}{4} - 2m\mu}\right) e^{-\frac{m}{2}f_0^2 r}, & \text{for } 0 < \mu < m\frac{f_0^4}{8}, \end{cases} \qquad (19)$$

where $J_n(x)$, $I_n(x)$ are Bessel and modified Bessel functions.

We note that it may seem possible to construct additional zero modes in the following way. Instead of the ansatz of a rotationally invariant $u(r)$ just before Eq. (15), we could have chosen an ansatz

$$u(r, \varphi) = u_\alpha(r)\ e^{i\alpha\varphi} + u_{-\alpha}(r)\ e^{-i\alpha\varphi}. \qquad (20)$$

Then two second order differential equations follow relating these two functions. Generally there are four solutions to these equations. Boundary conditions at the origin $r = 0$ select a subset of two of these solutions. Boundary conditions at infinity select a different subset of two solutions. However, barring a coincidence, none of those solutions finite at the origin are also finite at infinity. Even if such coincidence arises for some special value of μ, by the above arguments, the additional zero modes must appear in topologically unprotected pairs, that will be split to finite $\pm E$ energies by a slight generic deformation of the potential (order parameter distortion). Hence we conclude that generically there will be no additional zero modes (except the one found above) for an odd-vorticity vortex.

Thus we indeed find that the number of zero modes in a symmetric odd-vorticity vortex must be one. Since a smooth deformations of the order parameter can only change the zero mode number by multiples of two, an arbitrarily shaped odd-vorticity vortex must have an odd number of zero modes. However, any number of zero modes other than one is not generic and will revert to one under an arbitrary deformation of the order parameter.

To summarize, the results presented here establish the robustness of the zero modes localized on well-separated ($r_{\text{separation}} \gg 1/(m\Delta)$) odd-vorticity vortices and support the idea that they can eventually be used to demonstrate non-Abelian statistics and perhaps even for quantum computation.

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